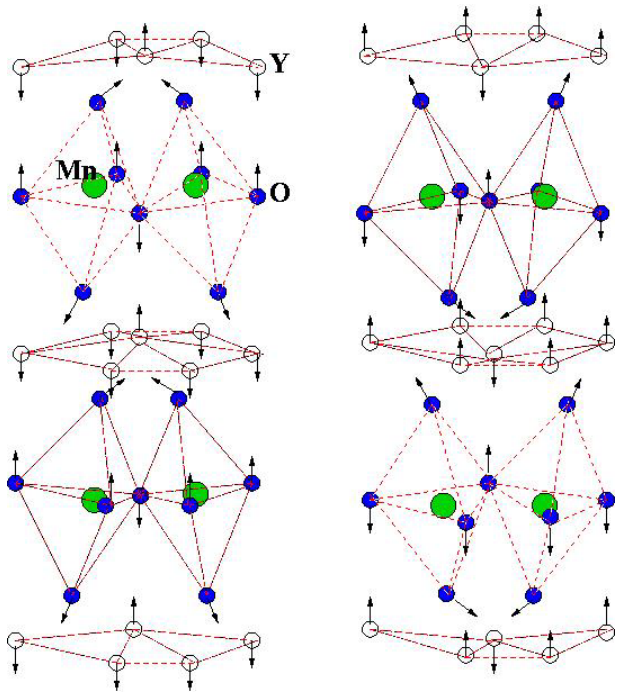
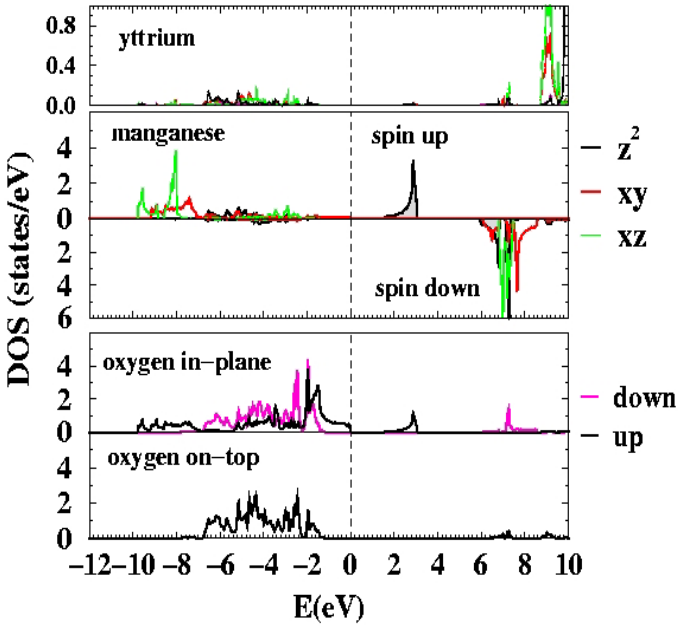
Computational design and optimization of novel multiferroics, Nicola Spaldin, UCSB, DMR-0312407



- $YMnO_3$ is unusual and potentially technologically important because it combines ferroelectricity with magnetic ordering
- We determined that the ferroelectricity originates from geometric rotations, rather than the rehybridization that usually occurs at ferroelectric phase transitions
- Therefore usual indicators of ferroelectricity do not hold:

The Born Effective Charges, which are anomalously large in conventional ferroelectrics, are close to the formal ionic charges:

The density of states (DOS), calculated using our pseudopotential self-interaction corrected density functional formalism, indicates minimal Y-O and Mn-O hybridization



Y +3.6, Mn +3.3, O_T −2.3, O_P −2.2

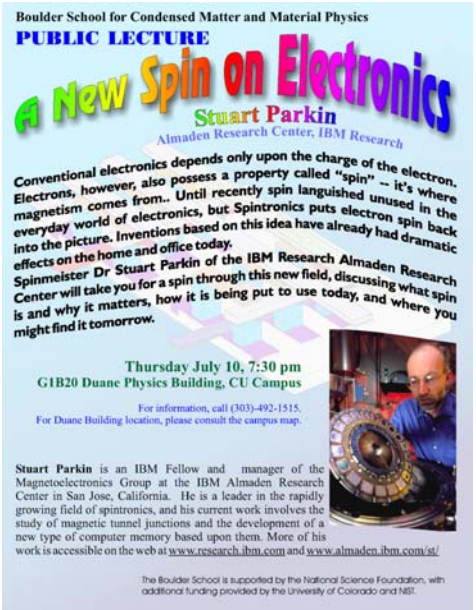
A. Filippetti and N.A. Spaldin, *Self-interaction-corrected pseudopotential scheme for magnetic and strongly-correlated systems*, Phys. Rev. B **67**, 125109 (2003)

B.B. van Aken, T.T.M. Palstra, A. Filippetti and N.A. Spaldin, *Origin of ferroelectricity in magnetoelectric $YMnO_3$*, Nature Materials **3**, 164 (2004)

Spaldin organized (with Dan Arovas and Anupam Garg) the 2003 Boulder School on Frontiers of Magnetism

Over 60 students from around the world worked with more than 15 teachers during the month-long school

A web-site:
http://research.yale.edu/boulder/Boulder-2003
was established with lecture notes, reading material, and other resources



Public lectures were presented by Stuart Parkin (IBM) and Frances Hellmann (UCSD)